Date of Issue:
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SAFETY DATA SHEET

1. Substance and Source Identification

Product Identifier

SRM Number: 1837
SRM Name: Methanol (9 volume percent) and t-Butanol (6 volume percent) Reference Fuel
Other Means of Identification: Not applicable.

Recommended Use of This Material and Restrictions of Use

This Standard Reference Material (SRM) is intended for use in calibrating of instruments and evaluating techniques used for the determination of methanol and t-butanol in gasoline. The reference fuel is a mixture of 91 % isooctane (2,2,4-trimethylpentane) and 9 % *n*-heptane (volume fractions). A unit of SRM 1837 consists of five twenty-milliliter ampoules, two of each solution.

Company Information

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2. Hazards Identification

Classification

Physical Hazard:	Flammable Liquid	Category 2
Health Hazard:	Acute Toxicity, Oral and Inhalation	Category 4
	Skin Corrosion/Irritation	Category 2
	Serious Eye Damage/Irritation	Category 2B
	STOT, Single Exposure	Category 1
	Aspiration Hazard	Category 1

Label Elements

Symbol

Signal Word

DANGER

Hazard Statement(s)

H225	Highly flammable liquid and vapor.
H302+H332	Harmful if swallowed or if inhaled.
H304	May be fatal if swallowed and enters airways.
H315+H320	Causes skin and eye irritation.
H370	Causes damage to central nervous system.

Precautionary Statement(s)

P210	Keep away from heat, sparks, open flames, hot surfaces. — No smoking.
P241	Use explosion-proof electrical, ventilating, and lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist, vapors, or spray.
P264	Wash hands thoroughly after handling.

P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves, eye protection, and protective clothing.
P301+P310	If swallowed: Immediately call a doctor.
P331	Do NOT induce vomiting.
P302+P352	If on skin: Wash with plenty of water.
P305+P351+P338	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332+P337+P313	If skin or eye irritation occurs: Get medical attention.
P304+P340	If inhaled: Remove person to fresh air and keep comfortable for breathing.
P312	Call a doctor if you feel unwell.
P362+P364	Take off contaminated clothing and wash it before reuse.
P403+P235+P233	Store in a well-ventilated place. Keep cool. Keep container tightly closed.
P405	Store locked up.
P501	Dispose of contents and container according to local regulations.

Hazards Not Otherwise Classified: None.

Ingredients(s) with Unknown Acute Toxicity: None.

3. Composition and Information on Hazardous Ingredients

Substance: Reference gasoline with added alcohol components.

Other Designations: Synthetic gasoline blend composed of 91 % isooctane and 9 % *n*-heptane by volume.

Hazardous Component	CAS Number	EC Number (EINECS)	Nominal Mass Concentration (%)
Reference Gasoline Components			
Isooctane	540-84-1	208-759-1	76
n-Heptane	142-82-5	205-563-8	8
Alcohol Components			
Methanol	67-56-1	200-659-6	10
t-butanol	75-65-0	200-889-7	6

4. First Aid Measures

Description of First Aid Measures

Inhalation: If adverse effects occur, remove to well-ventilated (uncontaminated) area. If breathing is difficult, qualified personnel may administer oxygen. If not breathing, qualified personnel should give artificial respiration. Seek immediate medical attention.

Skin Contact: Rinse affected skin with water for at least 15 minutes, then wash thoroughly with soap or mild detergent and water. If skin irritation persists, seek medical aid and bring the container or label.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Seek immediate medical attention.

Ingestion: Aspiration hazard. Do not induce vomiting. Contact local poison control immediately; if vomiting occurs, keep head lower than hips to prevent aspiration. If unconscious, turn head to side; get medical attention immediately.

Most Important Symptoms/Effects, Acute and Delayed: Aspiration hazard, harmful if swallowed, central nervous system depression, and may cause blindness.

Indication of any immediate medical attention and special treatment needed, if necessary: If any of the above symptoms are present, seek immediate medical attention.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Severe fire hazard. Vapor/air mixtures are explosive above the flash point. Vapors or gases may ignite at distant ignition sources and flash back. See Section 9, "Physical and Chemical Properties" for flammability properties.

Extinguishing Media

Suitable: Regular dry chemical, carbon dioxide, water, or alcohol-resistant foam.
Unsuitable: None listed.

Specific Hazards Arising from the Chemical: Not applicable.

Special Protective Equipment and Precautions for Fire-Fighters: Move container from fire area if it can be done without personal risk. Avoid inhalation of material or combustion by-products. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

NFPA Ratings (0 = Minimal; 1 = Slight; 2 = Moderate; 3 = Serious; 4 = Severe)

Health = 3 Fire = 3 Reactivity = 0

6. ACCIDENTAL RELEASE MEASURES

Personal Precautions, Protective Equipment and Emergency Procedures: Use suitable protective equipment; see Section 8, "Exposure Controls and Personal Protection". Keep out of waters supplies and sewers.

Methods and Materials for Containment and Clean up: Avoid heat, flames, sparks and other sources of ignition. Stop leak if possible without personal risk, with water spray to reduce vapors. Absorb spilled material with sand or non-combustible material and collect in appropriate container for disposal.

7. HANDLING AND STORAGE

Safe Handling Precautions: See Section 8, "Exposure Controls and Personal Protection".

Storage and Incompatible Materials: Store in a well-ventilated area. Keep separated from incompatible substances (see Section 10, "Stability and Reactivity").

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Exposure Limits			
Components	**OSHA (PEL)**	**ACGIH (TLV)**	**NIOSH (REL)**
Isooctane	No occupational exposure limits established.		
n-Heptane	TWA: 2000 mg/m^3 (500 ppm)	TWA: 400 ppm STEL: 500 ppm	TWA: 350 mg/m^3 (850 ppm) Ceiling: 1800 mg/m^3 (440 ppm) IDLH: 750 ppm
t-Butanol	TWA: 300 mg/m^3 (100 ppm)	TWA: 100 ppm	TWA: 300 mg/m^3 (100 ppm) STEL: 450 mg/m^3 (150 ppm) IDLH: 1600 ppm
Methanol	TWA: 260 mg/m^3 (200 ppm)	TWA: 200 ppm STEL: 250 ppm Skin[(a)]	TWA: 260 mg/m^3 (200 ppm) Ceiling: 325 mg/m^3 (250 ppm)[(b)] IDLH: 6000 ppm Dermal exposure[(c)]

[(a)] Skin – Potential significant contribution to overall exposure by the cutaneous route.
[(b)] 15 minutes.
[(c)] Potential for Dermal exposure.

Engineering Controls: Provide local exhaust or process enclosure ventilation system. Ensure compliance with applicable exposure limits.

Personal Protection Measures: In accordance with OSHA 29 CFR 1910.132, subpart I, wear appropriate Personal Protective Equipment (PPE) to minimize exposure to this material.

Respiratory Protection: If workplace conditions warrant a respirator, a respiratory protection program that meets OSHA 29CFR 1910.134 must be followed. Refer to NIOSH 42 CFR 84 for applicable certified respirators.

Eye Protection: Splash resistant safety goggles and emergency eyewash are recommended.

Skin and Body Protection: Chemical resistant clothing and gloves are recommended.

9. PHYSICAL AND CHEMICAL PROPERTIES

Note: The chemical and physical properties of components of the reference fuel are listed below.

Properties	Isooctane	*n*-heptane
Molar Mass (g/mol)	114.23	100.21
Molecular Formula	C_8H_{18}	C_7H_{16}
Appearance (physical state, color, etc.)	clear, colorless liquid	clear, colorless liquid
Odor	gasoline odor	gasoline odor
Odor threshold	not available	200 ppm
pH	not available	not available
Evaporation rate	<1 (ether = 1)	2.8 (butyl acetate = 1)
Melting point/freezing point	–107 °C (–161 °F)	–91 °C (–143 °F)
Specific Gravity (water = 1)	0.6919	0.6837
Density	not available	not available
Vapor Pressure	41 mmHg at 21 °C	40 mmHg at 20 °C
Vapor Density (air = 1)	3.9	3.45
Viscosity	not available	not available
Solubilities	water: immiscible; soluble in ether, alcohol, acetone, benzene, toluene, chloroform, xylene, carbon disulfide carbon tetrachloride, dimethylformamide, oils	water: 0.005 % soluble in ether, alcohol, acetone, chloroform.
Partition coefficient (n-octanol/water)	not available	not available
Thermal Stability Properties		
Autoignition Temperature	415 °C (779 °F)	205 °C (401 °F)
Thermal Decomposition	not available	not available
Initial boiling point and boiling range	99 °C (210 °F)	98 °C (208 °F)
Explosive Limits, LEL (Volume %)	1.1	1.05
Explosive Limits, UEL (Volume %)	6	6.7
Flash Point (Estimate)(closed cup)	–12 °C (10.4 °F)	–4°C (24.8 °F)
Flammability (solid, gas)	not available	not available

10. STABILITY AND REACTIVITY

Reactivity: Stable at normal temperatures and pressure.

Stability: X Stable _____ Unstable

Possible Hazardous Reactions: Not applicable.

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition. Minimize contact with material. Avoid inhalation of material or combustion by-products. Keep out of water supplies and sewers.

Incompatible Materials: Oxidizing materials, halogens, metal salts, acids, bases, combustible materials.

Hazardous Decomposition: Oxides of carbon.

Hazardous Polymerization: _____ Will Occur X Will Not Occur

11. TOXICOLOGICAL INFORMATION

Route of Exposure: X Inhalation X Skin X Ingestion

Symptoms Related to the Physical, Chemical and Toxicological Characteristics: Skin irritation, eye irritation, central nervous system depression, and may cause blindness.

Potential Health Effects (Acute, Chronic, and Delayed)

Inhalation: Acute exposure may result in irritation, headache, drowsiness, dizziness, vomiting, sleep disturbances, emotional disturbances, tremors, loss of coordination, visual disturbances, chest pain, difficulty breathing, irregular heartbeat, lung congestion, internal bleeding, blood disorders, kidney damage, liver damage, paralysis, brain damage, convulsions, unconsciousness, and coma. Chronic exposure may result in the same effects as acute exposure but with changes in body temperature, and changes in blood pressure.

Skin Contact: Acute exposure may cause irritation, skin disorders. Chronic exposure may cause irritation, skin disorders, tingling sensation, and allergic reactions.

Eye Contact: Exposure may result in irritation and other reversible effects.

Ingestion: Aspiration hazard. Exposure may cause the same effects as listed for inhalation.

Numerical Measures of Toxicity

Acute Toxicity: Category 4, Oral and Inhalation.

Components	Acute Toxicity	Acute Toxicity (point estimates)
Isooctane	Rat, Oral, LD50: >2500 mg/kg Rat, Inhalation, LC50: 47.7 mg/L (1 h)	Not classified.
n-heptane	Rat, Oral, LD50: 5000 mg/kg Rat, Inhalation, LC50: 103 g/m^3 (4 h) Rabbit, Skin, LD50: 3000 mg/kg	Not classified.
Methanol	Human, Oral LDLo: 143 mg/kg Rat, Oral, LD50: 5600 mg/kg Rat, Inhalation, LC50: 6400 ppm (4 h) Rabbit, Skin, LD50: 15800 mg/kg	Pure Methanol: Category 3 Oral, Inhalation and Dermal The guidance in OSHA's 1910.1200 Appendix A, Section A.1.3.3, (d) states that when only range data or acute toxicity hazard category information are available, to use the estimates listed in Table A.1.2. The values listed in the table for the Converted Acute Toxicity Point Estimates for Category 3 are: • Oral 100 mg/kg • Dermal 300 mg/kg • Inhalation: o Gases 700 ppmV o Vapors 3 mg/L o Dust/Mist 0.5 mg/L
t-Butanol	Rat, Oral, LD50: 2733 mg/kg Rat, Inhalation, LC50: 14100 ppm (4 h) Rabbit, Skin, LD50: >2000 mg/kg	Not classified.

The calculated data points for a 10 % methanol solution based on the Converted Acute Toxicity Point Estimates are: Oral 1000 mg/kg; Dermal 3000 mg/kg; Inhalation: Gases 7000 ppmV, Vapors 30 mg/L, Dust/Mist 5 mg/L.

Therefore, the mixture is classified as:
Acute Toxicity: Oral, Category 4; Inhalation, Dust/Mist: Category 4

Skin Corrosion/Irritation: Category 2; may cause irritation, redness, and defatting of the skin.

Serious Eye Damage/Irritation: Category 2B; may cause irritation with redness.

Respiratory Sensitization: No data available.

Skin Sensitization: No data available.
Individuals have reported sensitivity to some of the components.

Germ Cell Mutagenicity: No data available.
Isooctane, Mutagenic, Mouse: 500 mg/kg

Carcinogenicity: Not classified.

Listed as a Carcinogen/Potential Carcinogen ____ Yes X No

Isooctane, *n*-heptane, methanol, and *t*-butanol are not listed by IARC, NTP, and OSHA as a carcinogen/potential carcinogen.

Reproductive Toxicity: No data available; not classified.

STOT, Single Exposure: Category 1.
Causes damage to central nervous system.

STOT, Repeated Exposure: No data available; not classified.

Aspiration Hazard: Category 1. 2,2'4-Trimethylpentane and *n*-heptane are aspiration hazards.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data

Components	Aquatic Toxicity
n-heptane	Fish: Cichlid, LC50 (96 h): 375 mg/L
t-butanol	Fish: Fathead minnow, (*Pimephales promelas*), LC50 (96 h): 6130 to 6700 mg/L [flow-through] Algae: Pond scum, (*Desmodesmus subspicatus*), EC50 (72 h): >1000 mg/L Invertebrate: Water flea, (*Daphnia magna*), EC50 (48 h): 933 mg/L

Persistence and Degradability: No data available.

Bioaccumulative Potential: *t*-butanol BCF: 1.09 (fish)

Mobility in Soil: No data available.

Other Adverse effects: No data available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with all applicable federal, state, and local regulations. Subject to hazardous waste regulations US EPA 40 CFR 262.

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: UN1203; Gasoline; Hazard Class 3; Packing Group II.

15. REGULATORY INFORMATION

U.S. Regulations

CERCLA Sections 102a/103 (40 CFR 302.4): Isooctane: 1000 lbs (454 kg) final RQ.
Methanol: 5000 lbs (2270 kg) final RQ.

SARA Title III Section 302 (40 CFR 355.30): None of the components are regulated.

SARA Title III Section 304 (40 CFR 355.40): None of the components are regulated.

SARA Title III Section 313 (40 CFR 372.65): *t*-Butanol: 1 % de minimis concentration.
Methanol: 1 % de minimis concentration.

OSHA Process Safety (29 CFR 1910.119): None of the components are regulated.

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE HEALTH:	Yes
CHRONIC HEALTH:	No
FIRE:	Yes
REACTIVE:	No
PRESSURE:	No

State Regulations
California Proposition 65: Not listed.

U.S. TSCA Inventory: Isooctane, *n*-heptane, methanol, and *t*-butanol are listed.

T**SCA 12(b), Export Notification:** Not listed.

Canadian Regulations: WHMIS Information is not provided for this material.

16. OTHER INFORMATION

Issue Date: 15 June 2015

Sources: ChemADVISOR, Inc., SDS *2,2,4-Trimethylpentane*, 20 March 2015.

ChemADVISOR, Inc., SDS *n-Heptane*, 20 March 2015.

ChemADVISOR, Inc., SDS *Methyl Alcohol*, 20 March 2015.

ChemADVISOR, Inc., SDS *Tert-Butyl Alcohol*, 20 March 2015.

Key of Acronyms:

ACGIH	American Conference of Governmental Industrial Hygienists	NTP	National Toxicology Program
CAS	Chemical Abstracts Service	OSHA	Occupational Safety and Health Administration
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act	PEL	Permissible Exposure Limit
CFR	Code of Federal Regulations	RCRA	Resource Conservation and Recovery Act
DOT	Department of Transportation	REL	Recommended Exposure Limit
EINECS	European Inventory of Existing Commercial Chemical Substances	RQ	Reportable Quantity
EPCRA	Emergency Planning and Community Right-to-Know Act	RTECS	Registry of Toxic Effects of Chemical Substances
IARC	International Agency for Research on Cancer	SARA	Superfund Amendments and Reauthorization Act
IATA	International Air Transportation Agency	SCBA	Self-Contained Breathing Apparatus
IDLH	Immediately Dangerous to Life and Health	SRM	Standard Reference Material
LC50	Lethal Concentration	STEL	Short Term Exposure Limit
LD50	Median Lethal Dose or Lethal Dose, 50 %	STOT	Specific Target Organ Toxicity
LEL	Lower Explosive Limit	TLV	Threshold Limit Value
MSDS	Material Safety Data Sheet	TPQ	Threshold Planning Quantity
NFPA	National Fire Protection Association	TSCA	Toxic Substances Control Act
NIOSH	National Institute for Occupational Safety and Health	TWA	Time Weighted Average
NIST	National Institute of Standards and Technology	UEL	Upper Explosive Limit
n.o.s.	Not Otherwise Specified	WHMIS	Workplace Hazardous Materials Information System

Disclaimer: Physical and chemical data contained in this SDS are provided only for use in assessing the hazardous nature of the material. The SDS was prepared carefully, using current references; however, NIST does not certify the data in the SDS. The values for this material are given in the NIST Certificate of Analysis.

Users of this SRM should ensure that the SDS in their possession is current. This can be accomplished by contacting the SRM Program: telephone (301) 975-2200; fax (301) 948-3730; e-mail srmmsds@nist.gov; or via the Internet at http://www.nist.gov/srm.